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Abstract

An atomic-integral direct linear respons coupled cluster singles and doubles (CCSD) model to calculate triplet excitation energies is presented. The excitation space is parametrized in terms of excitation operators that are explicit coupled to triplet spin.

The triplet excitation spectrum of benzen is calculated in a basis ranging from 147 to 432 basisfunctions. The calculated triplet excitation energies are compared with experimental and other theoretical values.

Preliminary results will be presented for porphin with up to 678 basisfunctions.